Exceptional People Producing Great Science

With passion and skill, postdoctoral researchers apply their talents to the Laboratory's scientific and technical endeavors.

WANTED: Postdocs looking to pursue careers in science and technology. Must be willing to excel and expand their horizons by working with experts and contributing to world-class research. Opportunity awaits at Lawrence Livermore National Laboratory.

In any given year, Livermore is home to 110 to 150 postdoctoral researchers. Known as postdocs, these exceptional people—physicists, chemists, biologists, engineers, and mathematicians, to name a few—lend their scientific expertise to programs across the Laboratory. They come from all over the country and in some cases from abroad within the first five years after receiving a doctoral degree. As part of the Laboratory's Postdoc Program, they get hands-on experience while working closely with scientific leaders and colleagues in their chosen disciplines.

Typically, postdocs apply online for open positions in one of Livermore's four mission-related principal directorates: Science and Technology, which includes Computation, Engineering, and Physical and Life Sciences; Global Security; Weapons and Complex Integration; and National Ignition Facility (NIF) and Photon Science. Ultimately, candidates are selected for their knowledge and capabilities. "These assignments last approximately two years with the possibility of being extended to a third year," says Kris Kulp, director of the Institutional Postdoc Program Board, which oversees the program. After this initial term, some postdocs remain on the scientific staff at the Laboratory, while others head out into academia or industry. "Although we often want our postdocs to stay," says Kulp, "our basic goal is to provide an experience that prepares them well for any job they may have in the future."

Postdocs are integral to the complex work performed at the Laboratory. Almost 80 percent of these researchers receive support from the Laboratory Directed Research and Development (LDRD) Program, which applies internal research and development funds to forward-thinking, potentially high-payoff projects at the forefront of science. Their projects range from predicting California's future climate, supporting stockpile stewardship, and uncovering the secrets of the cosmos to building quantum computers, improving damage mitigation processes for laser optics, characterizing bacteria and spores, and revealing rare particle decays. Their work contributes to the Laboratory's important missions, and they bring a vibrancy and zeal to their research that only improves their chances of success. Says Kulp, "Postdocs have the energy, spark, and enthusiasm that gets translated into great science."

Building California's Climate Record

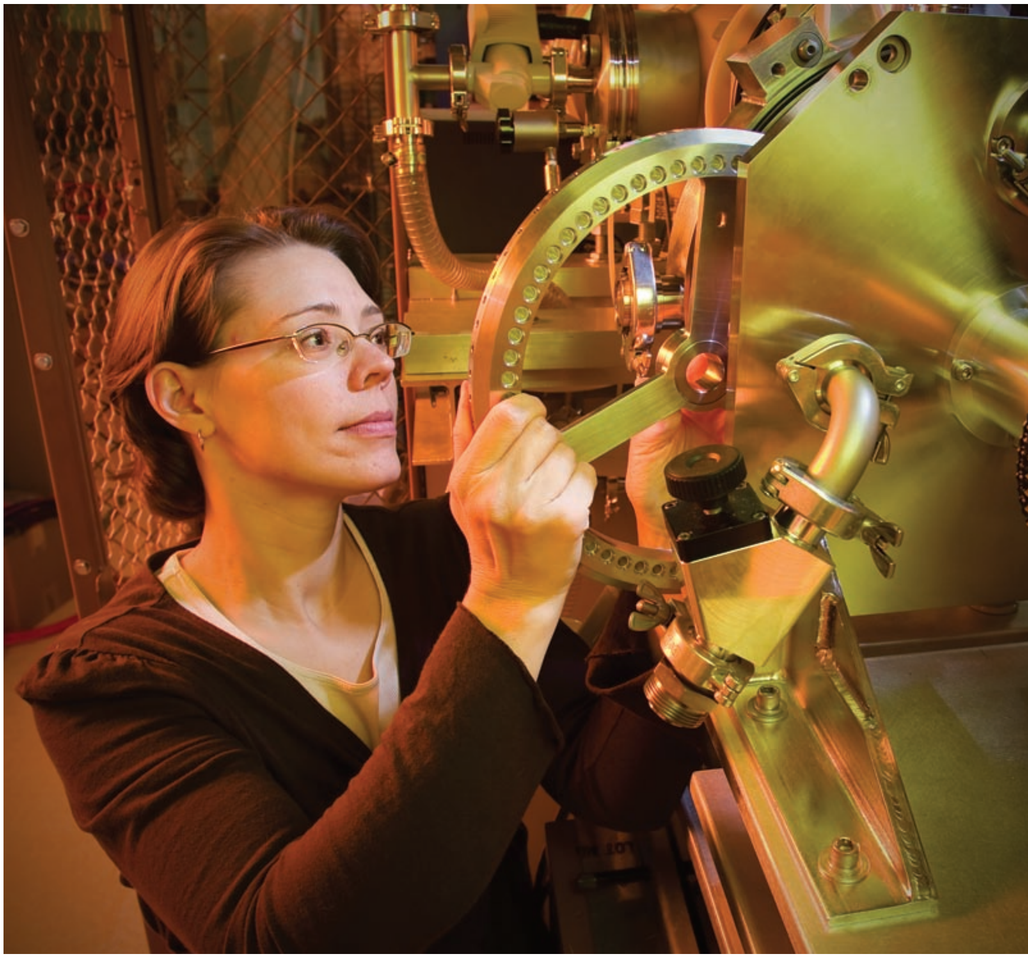
As part of the Laboratory's efforts to predict future climate change, Susan Zimmerman is spearheading a project to develop high-precision paleoclimate records for use in regional climate models. Current models typically use data for only the last 150 years and, thus, miss wet and dry periods from past millennia.

"Remarkably, over the last century, the West has been relatively wet compared to the average for the last 2,000 years," says Zimmerman, who received a Ph.D. in earth sciences from Columbia University. "Without more long-term data, predictive modeling is biased toward these anomalously wet conditions."

With funding from the LDRD Program, Zimmerman is working with researchers across California to analyze lake sediments and develop records that span the last two millennia. "Lakes are long-lived, wet areas where materials are continually deposited over time," she says. Data from these records will be used to map previous drought patterns in California and help climate modelers more accurately simulate the range of natural climate changes. With this information, state agencies can determine the infrastructure needed to meet future demands for water.

"An important part of my effort is building a network of collaborators who are already working on paleoclimate records in different areas of the state," says Zimmerman. She and her colleagues collect samples from natural outcrops such as stream cuts or fault scarps or from vertical cores of sediment extracted from a basin. Layers in the core indicate the conditions under which the sediment was deposited.

Zimmerman analyzes samples at the Laboratory's Center for Accelerator Mass Spectrometry, where she works with Livermore scientists Tom Guilderson, Tom Brown, and Graham Bench, the center's director. Zimmerman pretreats each sample, which may be charcoal, pine needles,

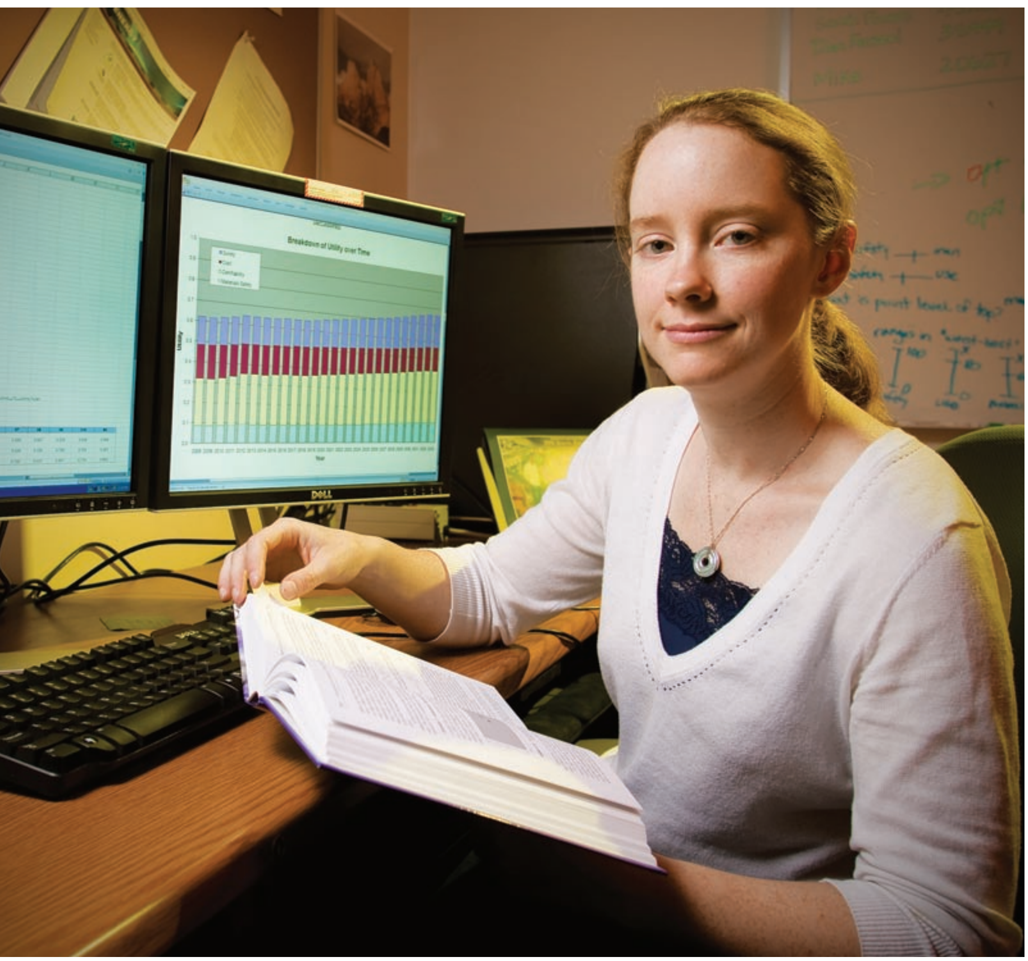


Susan Zimmerman loads a sample wheel into the ion source of an accelerator mass spectrometer.

or other macrofossils; combusts it into carbon dioxide gas; and then catalyzes the gas into graphite powder. The powder is pounded into aluminum sample targets, which are arranged with standard targets and blanks in a sample wheel and loaded into the spectrometer. A wheel with up to 50 unknown samples takes 8 to 12 hours to analyze, and the Laboratory's Natural Carbon Group, which includes Zimmerman, runs 2 to 3 wheels a week. With the high-precision accelerator mass spectrometer, Zimmerman can determine a sample's radiocarbon age to within 20 years.

Once the radiocarbon dates are calibrated to calendar years, Zimmerman and her colleagues establish a chronology for the paleoclimate records from the original core or outcrop. This record is then compared to other sources of ancient climate information, such as tree rings, to develop a regional picture. Combining well-dated paleoclimate records from statewide sites, Zimmerman will create time-slice maps of wet and dry patterns in California in 100-year intervals. In the last phase of her project, she will analyze spectra of the paleoclimate records to look for influences from mechanisms such as the El Niño climate pattern and the Pacific Decadal Oscillation, the long-term surface fluctuation of the Pacific Ocean.

"The Laboratory offers me the opportunity to work with many people in my field," says Zimmerman. This relationship with colleagues benefits everyone involved. Not only does Zimmerman get to do field work in new places and handle a variety of samples, but she also provides researchers statewide with data that might otherwise not be available to them. In addition, the data collected in her project will help strengthen the Laboratory's climate model predictions. With improved models, decision makers can better prepare for what research indicates will be a drier California in the next several decades.



Carol Meyers provides mathematical modeling expertise to several Laboratory programs.

Determining Cause and Effect

Although a native of the San Francisco Bay Area, Carol Meyers never thought her studies in operations research would lead to a career at a nuclear weapons laboratory. Prior to earning a Ph.D. from the Massachusetts Institute of Technology, Meyers spent two summers working with the National Security Agency in Maryland. While there, she began applying her skills to government projects, which led to her joining the Laboratory two-and-a-half years ago. She has since contributed to projects for Weapons and Complex Integration and Global Security and has spent time on LDRD-funded research. "I enjoy being involved in multiple areas of the Laboratory," says Meyers. "I have a lot of flexibility to work on different projects and that has been fun for me."

Working with Livermore scientists Cliff Shang, John Lathrop, Victor Castillo, and Lee Glascoe, Meyers applies mathematical modeling to help evaluate critical decisions. For example, she recently generated cost–benefit models that compare options associated with the National Nuclear Security Administration's (NNSA's) efforts to transform the nuclear weapons complex. "Such modeling illustrates how different choices can affect the complex as a whole," says Meyers, "and, thus, helps NNSA make decisions regarding the nuclear enterprise."

To develop the models, Meyers and her colleagues consult with relevant decision makers to understand the problem being addressed. In a stockpile cost model, one issue concerned whether to fix, replace, or dismantle different types of warheads before they reach the end of their lifetimes. The team identified the problem's variables and any limitations, such as the costs associated with each action, the yearly overall maintenance for a warhead type, and the maximum allowable cost. "Once we have the variables, we establish an objective, for instance, minimizing overall maintenance," says Meyers. Specialized mathematical computer programs then process the data and provide results.

In another project, called MARS (Modeling the Adversary for Responsive Strategy), Meyers is helping Global Security assess different countermeasures against terrorist activity. The MARS model incorporates intelligence data and output from systems such as the Joint Conflict and Tactical Simulation. (See *S&TR*, April/May 2009, pp. 16–22.) "We try to find out who the bad guys are, determine their motivations, and quantify damages that could result from a possible attack," says Meyers. "We then use these data to gauge the effectiveness of countermeasures." This work is related to Meyers's efforts on an LDRD project to model higher adaptive systems in which adversaries change their behavior in response to detection or prevention activities.

Meyers's enthusiasm for her work is palpable. She finds her projects challenging and welcomes the opportunity to learn more, such as participating in the Weapons Intern Program at nearby Sandia National Laboratories. "People at Livermore and Sandia understand the need to pass important knowledge and skills to the next generation of scientists," says Meyers, who plans to join the Laboratory's scientific staff once she completes her postdoc term.

"I never thought I would be involved in this kind of work," she says. "Coming from a liberal background, my family and friends were shocked that I decided to work for a nuclear weapons laboratory. However, I explain that what I am doing is helping to secure a smaller, safer, and more reliable nuclear weapons complex."

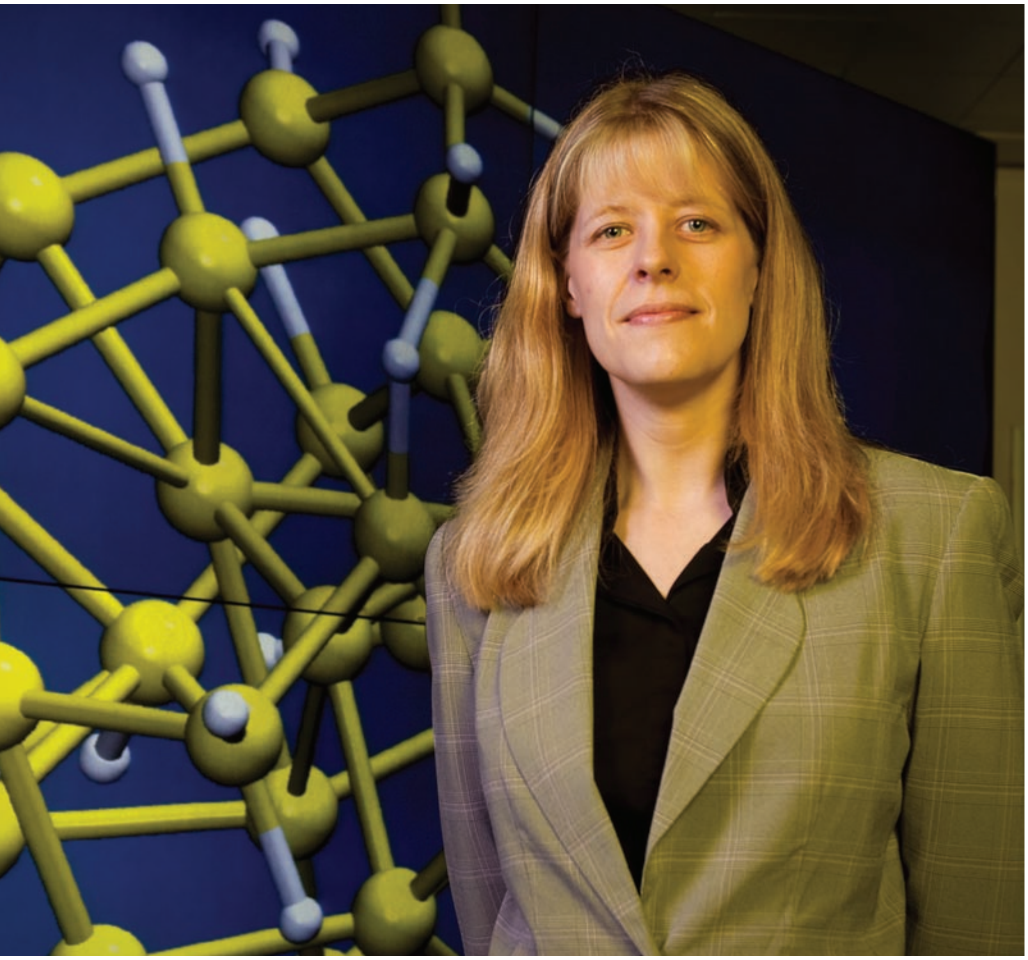
Andrew Cunningham applies three-dimensional modeling to simulate the formation of high-mass stars.

The Life of a Star

Livermore scientists have long been interested in understanding the origins of the universe and celestial bodies such as stars and other solar systems. Andrew Cunningham, who received a Ph.D. in astrophysics from the University of Rochester, is helping researchers improve their understanding of these complex stellar phenomena. Like other postdocs at the Laboratory, Cunningham works on multiple projects. In one project, he uses three-dimensional (3D) models to simulate the formation of stars whose masses are over 20 times greater than that of the Sun.

Star formation begins when a protostellar core draws in gases as it rotates about its axis. Eventually, the dense core collapses into a rapidly rotating accretion disk, similar to the way figure skaters spin faster as they bring their arms closer to their bodies. Gas falls through the disk and feeds the nascent star growing at the disk's center. As a result, gravitational attraction increases, and the star becomes more massive. Throughout this process, radiation emitted from the star's core is pushed outward, opposing the force of gravity and slowing accretion.

Unlike their low-mass counterparts, high-mass stars achieve thermonuclear burn while they are still accreting. Once a star grows to 20 times the mass of the Sun, the outward radiation force becomes strong enough to overcome the inward



Heather Whitley uses the Laboratory's advanced computing resources to study nanomaterials.

gravitational pull. "Researchers expected this process to stop accretion and limit stellar mass to at most 20 times that of the Sun," says Cunningham. "However, stars more than 100 times the Sun's mass have been observed—a phenomenon that is difficult to explain." Simulations by Cunningham, Livermore physicist Richard Klein, and collaborators Christopher McKee from the University of California (UC) at Berkeley and Mark Krumholz from UC Santa Cruz indicate that fluid instabilities in the core free radiation to move outward while still allowing gases to reach the disk.

Previous researchers produced 2D simulations that depicted the rotation of the star and the effects of the accretion disk. "In 2D, we could see how the star collapses and the disk builds and then shields itself from the radiation, creating a gas-scattering phenomenon toward the poles," says Cunningham. The 3D simulations indicate that this gas around the axis inflates radiation-filled bubbles and pushes them out from the core. The bubbles' walls capture the gas and become a mechanism for moving it into the accretion disk.

In 3D, Cunningham and his colleagues can observe gravity, radiation, and fluid dynamics interacting to create these massive stars. In addition, because 3D simulations can depict asymmetric processes, the team can see how fragments of the accretion disk become a binary star within the core and how this second star affects the formation of the high-mass star.

Cunningham runs simulations on the Datastar system at the San Diego Supercomputer Center, using the ORION code. "We start by inputting a slow, rotating dense core of gas into the simulation," he says, "and evolve the system according to a mathematical description of physical processes." ORION applies a technique called adaptive-mesh refinement in which individual grid points, called voxels, are continuously refined as the simulation progresses, which improves grid resolution. "We achieve very high-fidelity results in 3D by concentrating the computational effort where it is most needed," says Cunningham. Focusing the simulation on specific areas of interest reveals gravitational, radiative, and hydrodynamic processes of star formation that would otherwise remain unseen.

For Cunningham, working at Livermore has enabled him to apply his knowledge of computation and astrophysics to a broader spectrum of research. "The Laboratory is conducting ambitious research," he says. "It's a privilege to be part of that work."

A Closer Look at Nanomaterials

Computer simulations also play a significant role in helping researchers understand the functions of materials and living organisms. Since arriving at the Laboratory a year and a half ago, postdoc Heather Whitley has worked with scientists Eric Schwegler and Tadashi Ogitsu using Livermore's advanced computing resources to study the properties of nanomaterials under pressure, the effects of surface structure on the x-ray absorption spectra of a nanomaterial, and materials designed for quantum computers.

Whitley received a Ph.D. in theoretical chemistry from UC Berkeley. Her initial research at the Laboratory focused on simulations of nanometer-size quantum dots—semiconductors with electrons that are spatially confined because of their small size. Her focus is on understanding how the size of a nanoparticle affects its structural phase transitions and optoelectronic properties, and whether those effects can be used in novel applications.

When a material shrinks to nanometer size (10^{-9} meters), its surface has an increased influence on its physical and optical properties as well as its crystalline structure. External conditions, such as applied pressure, further modify this structure. In a nanometer-size material, these changes can affect how the material functions in a particular application. Using quantum mechanical simulations, Whitley examined the size dependence of pressure-induced structural phase transitions in silicon quantum dots.

"Understanding fundamental properties at a microscopic level is key to developing new technologies based on semiconductor nanomaterials," says Whitley. In addition, she is collaborating with David Prendergast and other researchers from Lawrence Berkeley National Laboratory to calculate the x-ray absorption spectra of cadmium–selenium nanomaterials. Both of these studies will help scientists better understand the surface structure of nanomaterials on a microscopic level.

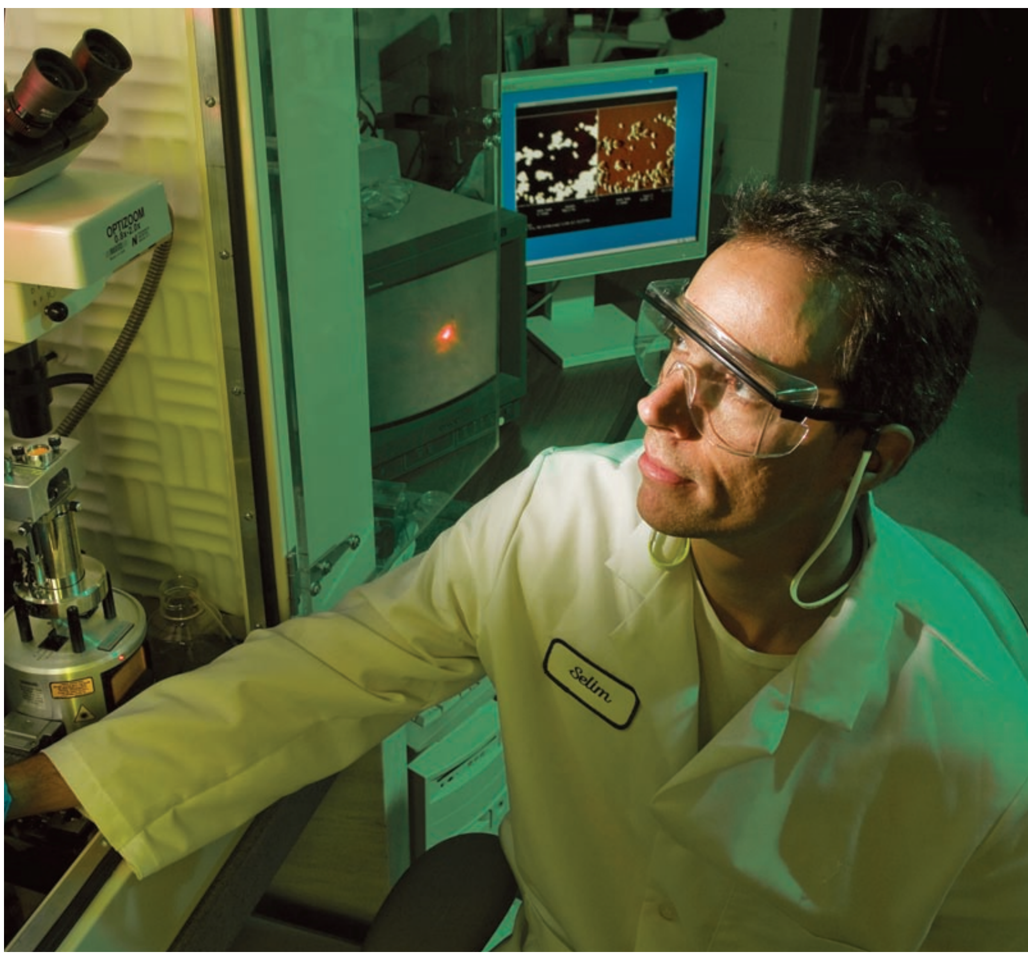
Whitley is also working with the Berkeley Quantum Information and Computation Center at UC Berkeley on a detailed computational analysis of materials for quantum computing. "A major barrier to developing quantum computers is decoherence, a process by which information encoded in a quantum state is lost because of interactions between the quantum system and its surroundings," says Whitley.

In an earlier project, the Berkeley group, which is led by professor K. Birgitta Whaley, used both the electron and nuclear spin states of a single phosphorus-31 donor atom in silicon to study an implementation of quantum computing. The group's findings suggest that the donor electron spin state, which has a fast response to an external field, could be used to perform fast quantum operations. Information encoded in the electron spin state could be transferred to the nuclear spin state, which has a longer lifetime, to enable efficient readout of quantum information. Collaborators at Lawrence Berkeley are also investigating the proposed design to determine which materials are suitable for building a quantum computer.

Working with professionals in her field has opened Whitley's eyes to its many possibilities. "I've seen what science is like outside academia," she says. "Plus, I've had an opportunity to use some of the most advanced computational equipment in existence. I don't think I could have ended up in a better place."

Understanding Crystal Growth

After receiving a Ph.D. in chemical engineering from Virginia Polytechnic Institute and State University (Virginia Tech), Selim Elhadj has spent the last three years at Livermore contributing to such diverse programs as NIF and biosciences. "I was brought to the Laboratory because of my knowledge of crystal growth processes, which are essential for understanding the structural dynamics of nonlinear optical materials and, surprisingly, biological membranes," says Elhadj. Using atomic force microscopy (AFM), he helped develop a method for mitigating damage on laser optics and characterized the dynamics of surface processes in spores and



Selim Elhadj's expertise in crystal growth processes supports a diverse range of Laboratory programs.

bacterial membranes exposed to different environmental perturbations.

In AFM, a nanometer-size pointed tip is moved across a substrate in a raster pattern. The amount of force on the tip changes as it passes over variations, such as scratches or elevated areas on the substrate's surface, which then deflect the tip. AFM records the deflections and reconstructs a complete topography of the surface.

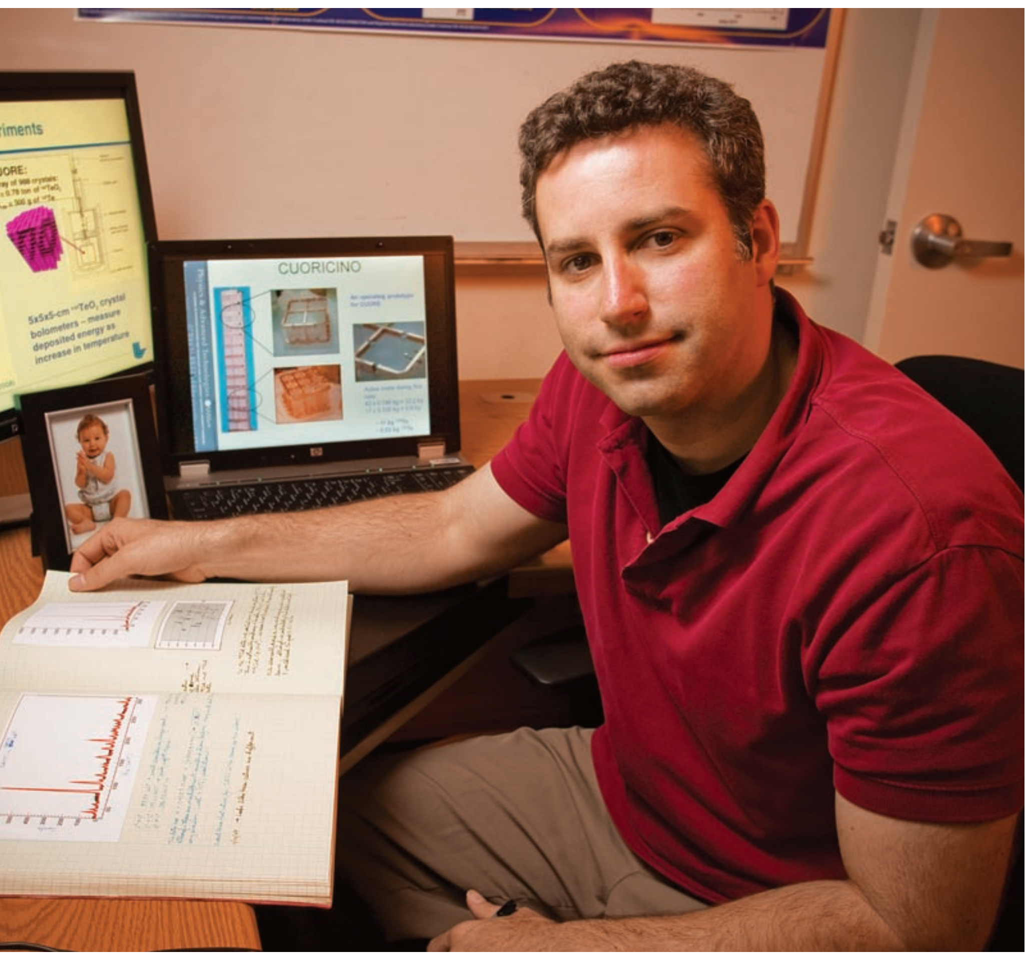
When a substrate is exposed to a solvent-containing atmosphere, a nanometer-thin layer of solvent and a meniscus form where the tip contacts the substrate surface. Elhadj and his colleagues discovered that this approach provides a mechanism by which ions within the material can be transported and redistributed to dissolve mounds and fill in grooves on a material's surface.

In an LDRD-funded study, Elhadj, Vaughn Draggoo, Alex Chernov, and Jim De Yoreo placed a laser-damaged potassium–dihydrogen–phosphate (KDP) crystal substrate into a tightly controlled atmosphere. As the meniscus passed over imperfections in the crystal, KDP molecules were dissolved from convex features and precipitated in concave ones. This redistribution of material was thermodynamically driven and well predicted by a form of the Gibbs–Thomson law, which relates surface curvature to vapor pressure and chemical potential. Says Elhadj, "The mitigation method relies on the shape-dependent solubility of the features, the contrast in their local solubility, and the molecular fluxes within the solvent layer."

Elhadj has also worked with Ibo Matthews and Steven Yang to research methods that will mitigate defects in silica optics by using lasers to melt and vaporize silica. "We used thermographic techniques to measure the temperature of the laser-exposed surfaces," he says. "We then included these measurements in models to predict how the optical materials change and to build diagnostic tools for process control. Measuring the temperature is essential because it represents the driving force of the observed changes relevant to laser-based mitigation."

In a project funded by the Department of Energy and other government agencies, Elhadj and Alex Malkin used AFM to characterize bacterial spores and study structural dynamics of cell surfaces at subnanometer resolution. "Bacteria derive many of their characteristics from their environment," says Elhadj. "We can measure their structures to deduce formulation signatures, for example, to determine if bacteria grew in their natural environment or were manufactured."

AFM is an excellent tool for studying extremely small organisms because spore formulation can be observed in vivo using high-resolution images. "AFM is the only technique that can provide structural information at the scales we are interested in and within relevant environments," says Elhadj. As a result of his efforts, Elhadj has helped expand AFM as a tool for mission-related applications. In doing so, he has deepened the Laboratory's understanding of complex biological crystal growth processes.



Lawrence Fellow Nicholas Scielzo is working on an international project to detect a rare decay process.

A Detector for a Rare Phenomenon

A small subset of postdocs comes to Livermore as part of the Lawrence Fellowship Program. (See *S&TR*, November 2002, pp. 12–18.) These individuals have the freedom to choose the projects they work on during their three-year term. One such postdoc is Nicholas Scielzo, who received a Ph.D. in physics from UC Berkeley. At the Laboratory, he splits his time between three nuclear physics projects, one of which involves detecting an extremely rare radioactive process known as neutrinoless double-beta decay.

In standard double-beta decay, two neutrons in a nucleus are converted to two protons, emitting two beta particles and two neutrinos that share the energy generated from the decay. In neutrinoless decay, the neutrinos annihilate each other instead of being emitted, and the full energy—a little over 2 megaelectronvolts—is carried away by the beta particles. "However," says Scielzo, "this decay can only occur if a neutrino and its antimatter, the antineutrino, are the same particle." In a project funded by the Department of Energy's Office of Science and LDRD, Scielzo is working with U.S. and Italian collaborators to build an extremely sensitive detector to identify this rare decay mode.

CUORE, the Cryogenic Underground Observatory for Rare Events, will be a 1-ton detector located within Italy's Gran Sasso mountain group. The detector will contain an array of nearly 1,000 tellurium dioxide crystals, each a 5-centimeter cube. Tellurium-130 is one of the few isotopes that emit two neutrinos through double-beta decay and thus could theoretically undergo the neutrinoless decay process. The crystals will be cooled to 0.01 kelvins above absolute zero using dilution refrigeration. "At this temperature, each crystal's heat capacity is small enough that the energy from a single radioactive decay within the crystal will be detected," says Scielzo. Sensitive thermometers outside the crystals will indicate a change in temperature, which the team will then use to calculate the decay energy.

As part of his research, Scielzo tests the raw materials used to make the crystals and the shielding for the detector. He also works with vendors to ensure that crystals meet the team's strict specifications. "We look for the most radio-pure materials, those with little to no radioactive background," says Scielzo.

Excess radioactive decay would overshadow the unusual signal they are trying to detect. The detector is surrounded by 1,400 meters of rock overburden to protect it from cosmic muons. Radio-pure shielding must be added to eliminate background radiation from the surrounding environment. Scielzo also applies his knowledge of particle physics to help CUORE researchers interpret the data from the device and develop new detection methods. "Currently, I am researching tellurium-120, which could also undergo the decay," says Scielzo.

CUORE must run for up to five years to collect enough data for accurate analysis. However, researchers on the project know that what they may find is well worth the wait. "The neutrinoless double-beta decay experiments at CUORE have the potential to reveal interesting properties of neutrinos that no other experiments have been able to show," says Scielzo. In addition to proving that the neutrino and its antimatter are the same particle, these experiments could help identify the neutrino mass hierarchy and scale and provide details to explain why matter dominates over antimatter in the universe. "The experiments won't tell us everything we want to know about the formation of our universe," says Scielzo, "but they could provide one component of the larger explanation."

A Mutually Beneficial Relationship

For decades, postdocs have lent their energy and talents to the Laboratory's scientific endeavors, and this tradition will continue into the foreseeable future. Through the Postdoc Program, researchers can apply their skills and expand their knowledge, and the Laboratory maintains a valuable mechanism for recruiting talented scientists and engineers. "The high-quality work of our postdocs enhances the great science performed at the Laboratory," says Kulp. "We are always mindful of how lucky we are to have them working here." They truly are exceptional people producing great science.

—*Caryn Meissner*

Key Words: accelerator mass spectrometer, atomic force microscopy (AFM), climate change, Cryogenic Underground Observatory for Rare Events (CUORE), high-mass star, Institutional Postdoc Program Board, mathematical modeling, nanoparticle, National Ignition Facility (NIF), neutrinoless double-beta decay, particle physics, quantum computing, stockpile stewardship.

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